```
T F F F 1 3 3 VCHK, TEST, LSPINS, LSURF, NRUN, LPR, LDU
1
 2
      Cu
3
                               (TRUE MEANS COMPLEX SECULAR EQUATIONS)
      7.00
 4
5
     99
     -.0000
               0.5000
                        0.5000
6
7
      0.5000
               -.0000
                        0.5000
                        -.0000
8
      0.5000
               0.5000
9
              KINDS OF INEQUIV. ATOMS
10
       ICORR=2
                XALPH= 0.6666666
                                                              2=H-L
11
       350 29.00 2.10000 0.03
12
       1
             ATOMS
13
      0.00
              0.00
                     0.00
       7
14
15
       1 -1
      2 -1
16
17
      2 1
18
       2 -2
19
      3 -1
20
      3 1
      3 -2
21
22
                CFFT INDICES
23
    16.500
              7.0
                             SCMAX, RKMIX FOR V(R), RHO(R)
24
            HERE F= SPCGRP IN CART. COORDS.
25
     1 8 8 8
                  # SYM. KINDS, LMAX
26
      95 95 95
27
     POT8=F, EIGEN ONLY=F, TAPE66=F, DISP=F, TRIA=F, INITC=T
28
             0
                   11.
                          0.002
                                  0.00
        1
                                                     NW, NWSC, ZFILL, TKB
29
       -2.0
                1.10
                                           ELO, EHI
30
                0.00
                              99. 3
          0.60
31
             -4.40 0.50
32
       -1
33
       8.000
                              RKMAX
34
        0
35
     LSPEC=T,LINFOK=F
36
             8
         8
37
     TFTTTFFF DCOR, LHAM2, RLA, SDCOR, VRLA, PRES, FORC, AFRUN
38
     LSPNOR=F 180 LSOVEC=T LNCLSO=TTT 180=NSOBNDS
39
              ATOMCD, DCORMT
40
        5
                LMAX IN <V(NMT)>
41
                         NMAX IN MULTIPOLE EXP.
                 9
42
     43
     FRCOR=F,TOTAL=T,FRZQR=F,FRZQZ=F,HFIELD=0.000,SWSP=F,BMU=0.000,SPINF=1.0
44
     CRAY=F, BCS.COMPUT=F
     -0.000 0.000
45
46
           0
```

Instructions for INFILE File Input to LAPW Code

Ruler

123456789012345678901234567890123456789012345678901234567890 10 20 30 40 50 60 70

Note: This file is formatted. Every column position matters.

Line 1

T F F F 1 3 3 VCHK, TEST, LSPINS, LSURF, NRUN, LPR, LDU

123456789012345678901234567890123456789012345678901234567890

VCHK, TEST, LSPINS, LSURE, NRUN, LPR, LDU

PTIOE1.F: FORMAT (4(1X,L1),315)

VCHK = .TRUE. DISPLAY CONTINUITY OF COULOMB POTENTIAL ON BOUNDARIES

TEST = .TRUE. TEST MODE ON

= .FALSE. TEST MODE OFF

LSPINS = .TRUE. SPIN-POLARIZED CALCULATION

= .FALSE. NON-SPIN-POLARIZED

LSURF =.TRUE. ISOLATED SLAB CALCULATION FOR SURFACE

= .FALSE. BULK BAND STRUCTURE CALCULATION

NRUN = ID-number of present run

LPR = OUTPUT PRINT LEVEL

- = 0 MINIMUM OUTPUT
- = 3 MAXIMUM OUTPUT
- = 5 REANALIZED POTENTIAL IS CALCULATED USING A SLOW BUT ACCURATE WAY (I.E. THE DIRECT METHOD).

LPR.GE.4.AND.VCHK

PLANE WAVE CONTRIBUTION TO THE TOTAL ENERGY IS CHECKED BY A SLOW DOUBLE SUMMATION METHOD.

LDU = DUMP LEVEL (TAPE11, UNFORMATTED)

- = -2 N,L-LIKE CHARGE FOR EACH STATE ALSO ABOVE E-FERMI NOT COMPATIBLE WITH TOTAL ENERGY = T
- = 3 STANDARD CASE: DUMP COEFFICIENTS OF PSEUDO CDN, COULOMB POTENTIAL, TOTAL POTENTIAL, VALENCE- AND TOTAL DENSITIES. USED FOR TOTAL ENERGY CALCULATION
- = 4 ONLY VALENCE CHARGE DENSITY IS CALCULATED AND WRITTEN TO CDN1 FILE.
- = 5 VWORK WILL BE CALLED

LSPINS = .TRUE. SPIN-POLARIZED CALCULATION

= .FALSE. NON-SPIN-POLARIZED

Note: use LDU=-2 for DOS, and also when calculating energy bands.

Cu

1234567890123456789012345678901234567890123456789012345678901234567890

NAME

PTIOE1.F: FORMAT (A80)

This is a comment line that is printed on output files.

Line 3

```
F (TRUE MEANS COMPLEX SECULAR EQUATIONS)

12345678901234567890123456789012345678901234567890

LHRM

PTIOE1.F: FORMAT (4(1X,L1),3I5)

Inversion summertur, no inversion (complex secular equations)
```

Inversion symmetry: T = no inversion (complex secular equations)

F = inversion (real secular equations)

Line 4

7.00

123456789012345678901234567890123456789012345678901234567890 SCALE

PTIOE1.F: FORMAT(5D10.3)

Scale factor (this multiplies basis vectors for unit cell) - often this is a lattice constant

Line 5

99

123456789012345678901234567890123456789012345678901234567890

LATTIC, LATTYP

RDLAT.F: FORMAT (I3,A77)

Label for special lattices

Normally 99 for most lattices

hex = 2

BCC = 4

BCT = 7, 8, 9?

If LATTC = 4, special treatment for hexagonal lattice

Lines 6-8

```
-.0000 0.5000 0.5000 a-vector
0.5000 -.0000 0.5000 b-vector
0.5000 0.5000 -.0000 c-vector
```

((AVEC(I,J),I=1,3),J=1,3) RDLAT.F: FORMAT (3F10.6)

D. C. C. L. H. C. L.

Basis vectors for unit cell in Cartesian coordinates

Multiply these numbers by scale factor (see above) to get real values (in bohrs)

1 KINDS OF INEOUIV. ATOMS

123456789012345678901234567890123456789012345678901234567890

PTIOE1.F: FORMAT (215,F10.5)

Number of inequivalent atoms in the unit cell

Line 10

ICORR=2 XALPH= 0.6666666

2=H-L

123456789012345678901234567890123456789012345678901234567890

ICORR,XALPH,DLAMDA,IGRAD

PTIOE1.F: FORMAT(9X,I1,10X,F10.0,10X,F10.0,I10)

Exchange-correlation options

ICORR = 2 is Hedin-Lundquist

Use a value of 4 in column 60 to get Perdew 1991 GGA potential

Original Perdew-Wang = 1

Langreth-Mehl = 3

91 Perdew-Wang = 4

Note: Make_maz may use better subroutines for GGA, and make it more stable.

GGA potential will never be as continuous as LDA due to noise from interstitial region.

Because of convergence problems with GGA, may need to cut down mixing, and iterate longer.

If you use GGA, you will probably also have to increase the FFT by one, since the interstitial region is problematic (not the muffin-tin atom)

GGA potential will never be as continuous as LDA due to noise from interstitial mesh.

GGA may be more sensitive, you may need to cut mixing down and iterate longer.

Line 11

```
350 29.00 2.10000 0.03
```

123456789012345678901234567890123456789012345678901234567890

This line begins a block of lines.

The number of blocks is the number of inequivalent atoms in the unit cell.

JRI(JATOM), ZATOM(JATOM), R(JATOM), DX(JATOM)

PTIOE1.F: FORMAT (15,3F10.5)

JRI = 350 = number of radial mesh points

350 is ok for normal calculations, use 500 for forces

ZATOM = 29.0 for Cu

R = 2.1 bohrs for muffin-tin radius

DX = 0.03 = grid spacing - don't change

Note: ultimate test of LAPW is to change sphere radii slightly – do results depend on this?

- There is no advantage with filling all space with spheres with this method (full close packing).
- Convergence is improved if smaller sphere sizes are used for simple metals, and hard atoms are made bigger (however, don't make one atom overly large compared to others)

1 ATOMS

123456789012345678901234567890123456789012345678901234567890

PTIOE1.F: FORMAT (3I3)

NQ = 1 = number of equivalent atoms for each atom type

Leave this line alone. If a system has several equivalent atoms, you just specify the position of the first atom. The code will use the symmetry operations to generate all the others. By looking at what it generated is one check of the correctness of the SPCGRP file.

Line 13

Line 14

7

123456789012345678901234567890123456789012345678901234567890

NC

PTIOE1.F: FORMAT (313)

Number of core orbitals (relativistic)

Lines 15-21

- 1 -1
- 2 -1
- 2 1
- 2 -2
- 3 -1 3 1
- 3 -2

123456789012345678901234567890123456789012345678901234567890

(NPRNC(J,JATOM),KAPPA(J,JATOM),J=1,NC)

PTIOE1.F: FORMAT (213)

One line for each core orbital:

N, κ = Principal Quantum Number, Kappa (relativistic notation)

```
Line 22
```

4 4 4 CFFT INDICES

1234567890123456789012345678901234567890123456789012345678901234567890

(MF(I),I=1,3)

PTIOE1.F: FORMAT (3I3)

Fast Fourier Transform

4 means 24; because of this, increasing this number is very expensive.

7 or 8 is usually the largest number used in one direction; the code will usually stop if this number is too small.

This number scales with the size of the system and the number of G's used; because of the powers of 2 involved, it is very expensive to increase this number.

Main convergence problem is with GGA, need to increase this number by 1 in this case.

For GGA calculations, the interstitial region and not the muffin-tin is where the problems occur. This is why increasing CFFT indices is important.

Note: Make_maz may use better subroutines for GGA, and make it more stable.

Line 23

16.500 7.0 SCMAX, RKMIX FOR V(R), RHO(R)

123456789012345678901234567890123456789012345678901234567890

SCMAX, RKMIX

LAPW.F: FORMAT (5F10.5)

SCMAX = cut-off of G-vectors for potential expansion in intersitial region;

should usually be about twice as big as RKMAX + something;

= minimum sphere size (in bohrs) * G_cutoff (in inverse bohrs)

RKMIX = is not used (dinosaur — ignore comments in code and elsewhere)

Line 24

F HERE F= SPCGRP IN CART. COORDS.

123456789012345678901234567890123456789012345678901234567890

RLCOOF

LAPW.F: FORMAT(11L1)

Line 25

1 8 8 8 # SYM. KINDS, LMAX

1234567890123456789012345678901234567890123456789012345678901234567890

NSYMKD, (MXLS(I), I=1, NSYMKD)

LATHRM.F: FORMAT (20(I2,1X))

1 = number of symmetry kinds

LMAX = for each symmetry kind, one additional column for each kind

(LMAX = 8 usually)

Line 26

95 95 95

123456789012345678901234567890123456789012345678901234567890

(JRINMT(N), N=1, NTYPE)

LATHRM.F: FORMAT(2613)

Number of mesh-points for warping inside spheres

95 = usually safe for total energies

500 = good value for forces

```
Line 27
```

POT8=F, EIGEN ONLY=F, TAPE66=F, DISP=F, TRIA=F, INITC=T

POT8.LEIG.T66.DISP.TRIA.INITCG

LAPW.F: FORMAT(5X,L1,12X,L1,8X,L1,6X,L1,6X,L1,7X,L1)

INITC = T means do a new start-up (used for going to a slightly different structure – paramagnetic case only)

This is ok even for self-consistent runs, since it will then just reproduce the old deck. However, it is unnecessary for self-consistency, and should probably be set to F.

For spin-polarized calculations, if this flag is T, the code expects a paramagnetic input deck. Set this variable to F for subsequent iterations that have a spin-polarized deck.

Line 28

1 0 11. 0.002 0.00 NW,NWSC,ZFILL,TKB

123456789012345678901234567890123456789012345678901234567890

NWNDW,NWNDSC,ZFILL,TKB,FMOM

PTIOE2.F: (2I5,3F10.6)

ZFILL = total number of valence electrons

TKB = temperature broadening (in Ry)

TKB = 0.002 is coarse

TKB = 0.001 for a converged deck

Last number = fixed magnetic moment (in bohrs) for spin-polarized fixed moment method

= 0.0 for self-consistent spin-polarized calculations

Line 29

-2.0 1.10 ELO,EHI

123456789012345678901234567890123456789012345678901234567890

E1(M), E2(M), Do loop over M=1, NWNDW

PTIOE2.F: FORMAT(5F10.6)

ELO and EHI set energy window for valence panel

Line 30

0.60 0.00 99. 3

1234567890123456789012345678901234567890123456789012345678901234567890

EL(1), EL(3), CONT, LDIFF(N); Do loop over N=1, NTYPE

PTIOE2.F: (3F10.0,I5)

This and next few cards are a block of input lines for each inequvalent atom.

They specify over-rides for E₁'s (also extra orbitals).

First two numbers are default values for E_i's (with respect to muffin-tin zero);

 $E_1 = 0.60$ is normal default, $E_1^{(2)} = 0.0$ is normal default for local orbitals

leave the 99. alone

4th number = 3 = number of extra orbitals (0=none; otherwise # of orbitals to l+1; 3=spd)

If you had a spin-polarized calculation, the line would read:

0.60 0.60 0.00 0.00 99. 3

(i.e., spin-up and spin-down values for each quantity)

```
Line 31
```

1 -4.40 0.50

123456789012345678901234567890123456789012345678901234567890

L1,(EL(JS),JS=1,JSPINS),(EL(JS+2),JS=1,JSPINS)

PTIOE2.F: FORMAT(I4,4F10.6)

One line for each over-ride.

First number (1) = l-value to over-ride

Second and third numbers are over-rides for E₁'s:

use E_1 for core state; $E_1^{(2)}$ for valence band

Note: -4.40 = 3 p state of Cu

Local orbitals reduce dependency on linearization parameters.

Use less local orbitals for smaller atoms (smaller Z)

Line 32

-1

123456789012345678901234567890123456789012345678901234567890 PTIOE2.F: FORMAT(I4.4F10.6)

Signals end of over-rides / end of block for each inequivalent atom.

Line 33

8.000 RKMAX

123456789012345678901234567890123456789012345678901234567890

RKM(M)

PTIOE2.F: FORMAT(5F10.6)

Controls number of G-vectors in basis

Safe cut-offs:

4.0 = for Al

5.0 = for Si

6.0 = O, Si, Al and simple metals

7.0 = Fl

9.0 = for transition-metals and actinides

There is an advantage in using small sphere sizes for simple atoms so that hard atoms can be bigger, which improves the convergence. However, there is no advantage in attempting to fill all space with spheres. Also, don't exagerate this tendency too much and make one atom overly big compared to others.

Line 34

NKV

123456789012345678901234567890123456789012345678901234567890

NKV(M).SFK

PTIOE2.F: FORMAT(I5,2F10.6)

K-point generation (i5 format)

0 or negative = automatic k-point generation

positive number = number of k-points to be input by hand

[used for plotting bands, e.g., Γ ---X; in this case also set LDU=-2]

For automatic k-point generation for plotting energy bands, set this number to 999.

Note: IF(SFK.LE.EPS) SFK=ONE

Line 35+

1 KPDIR

KPDIF

PTIOE2.F: FORMAT(I5,2F10.6)

Number of k-directions (only used when NKV=999)

Format = (i5)

ONLY INCLUDE THIS LINE IF NKV=999

Line 36+

100 0.00000 0.00000 0.00000 0.50000 0.50000

KD, (QKPT(I,NK+1,M),I=1,3), (QKPT(I,NK+KD,M),I=1,3)

PTIOE2.F: FORMAT(I5,6F10.5)

Keep one line for each direction (KPDIR).

(i5,6f10.5) => npts,ki(3),kf(3) => number points,intial and final point

(in units of reciprocal lattice vetor)

ONLY INCLUDE THIS LINE IF NKV=999

Line 35

LSPEC=T,LINFOK=F

123456789012345678901234567890123456789012345678901234567890

LSPEC(M),LINFOK

PTIOE2.F: FORMAT (515)

LSPEC = T means use special points, set to F for DOS

LINFOK = T means extra k-points will be added to the mesh (e.g., Γ).

REMOVETHIS LINE WHEN NKV=999

Line 36

8 8 8

1234567890123456789012345678901234567890123456789012345678901234567890

KPDIV1(M), KPDIV2(M), KPDIV3(M), KPST, KPEND

PTIOE2.F: FORMAT (515)

Mesh size for k-points - x, y, z (should be multiple of 2)

REMOVETHIS LINE WHEN NKV=999

TFTTTFFF DCOR, LHAM2, RLA, SDCOR, VRLA, PRES, FORC, AFRUN

123456789012345678901234567890123456789012345678901234567890

DCOR, LHAM2, RLA, SOCOR, VRLA, PRES, FORC, AFRUN

LAPW.F: FORMAT(11L1)

DCOR =.TRUE. TREATS OVERLAPPING CORE-STATES EXACTLY BY EXPANDING INTO PLANE WAVES AND LATTICE HARMONIC

=.FALSE. CONSTANT CORE-CHARGE DENSITY IN INTERSTITIAL

RLA =.TRUE. RELATIVISTIC CALCULATION (FULLY REL. FOR CORE AND SCALAR-RELATIVISTIC FOR VALENCE)

=.FALSE. NON-RELATIVISTIC CALCULATION

SOCOR =.TRUE. SPIN-ORBIT INCLUDE IN CORE STATES

=.FALSE. CORE STATES TREATED SCALAR-RELATIVISTICALLY

VRLA =.TRUE. VALENCE STATES ARE SCALAR-RELATIVISTIC

=.FALSE. VALENCE-ONLY STATES ARE NON-RELATIVISTIC

PRES =.TRUE. THE PRESSURE WILL BE CALCULATED

=.FALSE. NO PRESSURE CALCULATION

Note: pressures probably don't work, since formalism was not updated to include local orbitals

FORC =.TRUE. THE FORCE ON EACH NUCLEUS WILL BE CALCULATED

=.FALSE. NO FORCES CALCULATED

FLM FUNCTIONS, SET IN SUBR. SETBAS

IS CALLED AGAIN IN CDNLV1 (THIS OPTION

SAVES DISK SPACE)

AFRUN = T for Anti-Ferromagnetic Calculations

Line 38

LSPNOR=F 180 LSOVEC=T LNCLSO=TTT

180=NSOBNDS

123456789012345678901234567890123456789012345678901234567890

LSPNOR, NSOBN, LSOVEC, (LNCLSO(I), I=1, NTYPE)

LAPW.F: FORMAT (7X,L1,I5,8X,L1,8X,50L1)

LSPNOR = T for spin-orbit to be included

180 = NOSPBNDS = number of bands to be included in 2nd variation

Note: set this to a large value, and cut off things with the windows.

Energy windows apply to scalar-relativistic states.

LNCLSO = has one T/F value for each inequivalent atom

(specifies where spin-orbit is included for each atom)

Add more T values for more atoms.

Don't partially turn off spin-orbit for atoms.

- C LSPNOR=.T. IF SPIN-ORBIT IS TO BE CALCULATED AND INCLUDED
- C NSOBN = NUMBER OF BANDS TO BE INCLUDED IN S-O CALCULATION
- C .F. IF STANDARD S-O ROUTINE (SETSOH) IS DESIRED
- C —IGNORED— D. SINGH
- C LNCLSO(J)=.T. IF THE SPIN-ORBIT INTERACTION ON THE J-TH
- C ATOM IS TO BE INCLUDED
- C =.E IF THE J-TH ATOM IS A LOW-Z ATOM AND SPIN-
- C ORBIT NEED NOT BE INCLUDED

FF ATOMCD, DCORMT

ATOMCD,DCORMT

LAPW.F: FORMAT(11L1)

Usually ATOMCD = F for self-consistent runs

Set ATOMCD = T if overlapping charge densities are used to start run

Note: will also need to set INITC = T for calculation to work correctly

Line 40

5 LMAX IN <V(NMT)>

(JMV(NW),NW=1,NWNDW)

LAPW.F: FORMAT(2015)

Line 41

9 9 9 NMAX IN MULTIPOLE EXP.

123456789012345678901234567890123456789012345678901234567890

(NCV(N),N=1,NTYPE) LAPW.F: FORMAT(2015)

Line 42

123456789012345678901234567890123456789012345678901234567890

ITMAX, (QMIX(I), I = 1, MIN(ITMAX, 9))

LAPW.F: FORMAT (BN,I2,F5.3,8F6.3)

6 = number of iterations

4.15 = 4 (Broyden) [use 0 for straight mixing]

15 = start-up percentage of mixing

10 columns (numbers) of type 4.15 [one for each iteration]

Line 43

FRCOR=F,TOTAL=T,FRZQR=F,FRZQZ=F,HFIELD=0.000,SWSP=F,BMU=0.000,SPINF=1.0

123456789012345678901234567890123456789012345678901234567890

FRCOR, TTL, FRZQR, FRZQZ, HFIELD, SWSP, BMU, SPINF

LAPW.F: FORMAT(6X,L1,3(7X,L1),8X,F5.3,6X,L1,5X,F5.3,7X,F4.1)

H-Field = magnetic field in Ry

Line 44

CRAY=F, BCS.COMPUT=F

LCRAY,LBCS

LAPW.F: FORMAT(5X,L1,12X,L1,8X,L1,6X,L1,6X,L1,7X,L1)

Line 45

-0.000 0.000

123456789012345678901234567890123456789012345678901234567890

(AFIELD(NN),NN=1,NTYPE)

LAPW.F: FORMAT (10F8.0)

H-Field and orbital symmetry when H-Field = 99 or -99

0 (

1234567890123456789012345678901234567890123456789012345678901234567890

(LFIELD(NN),NN=1,NTYPE) LAPW.F: FORMAT (1018)

H-Field and orbital symmetry when H-Field = 99 or -99

From: Matt Jones <mdj@sleipner.lanl.gov> To:rca@sleipner.lanl.gov Subject: symmetry lines in lapw Date:Thu, 6 Nov 1997 07:55:16 -0700 (MST)

I checked the method that I was using to compute energy bands along symmetry directions in Cu, since that was more familiar to me than Pu, and it looks fine. Here is a quick description of how you change the INFILE, to save you some time:

-from a converged calculation, set LDU=-2 to output QLMT file -3 lines following RKMAX value need to be changed to something like

999 1

100 0.00000 0.00000 0.00000 0.00000 0.50000 0.50000

the formats are:

(i5) - 999 => flag to do symmetry direction

(i5) - kpdir => number of directions

(i5,6f10.5) => npts,ki(3),kf(3) => number points,intial and final point

the ki and kf are in units of the reciprocal lattice vectors, so the above example does \Gamma-X in an fcc lattice. I also have a simple code to parse the QLMT file into a file containing a column directed list of up to 40 bands - it's in ~mdj/bin/qlm_parse.

Matt

From: David Singh <singh@dave.nrl.navy.mil>
To: rca@nidhug.lanl.gov, singh@dave.nrl.navy.mil
Cc: singh@slater.nrl.navy.mil
Subject: Re: Short Question

Date: Wed, 12 Nov 1997 13:12:20 -0500

Bob.

Sorry for the slow response. I've been out of town. The paramaters on the line for the charge density are SCMAX which controls the cut-off for the charge and potential and RKMIX which does nothing. It is an example of misleading comments in the input deck and INFO file — a dinosaur track. RKMAX several lines lower controls the cut-off for the basis set. Probably you should do convergence tests with respect to RKMAX. SCMAX is not a convergence parameter, but must be at least a small increment higher than twice RKMAX. RKMIX does nothing and may be left alone.

I hope that this is of help.

David